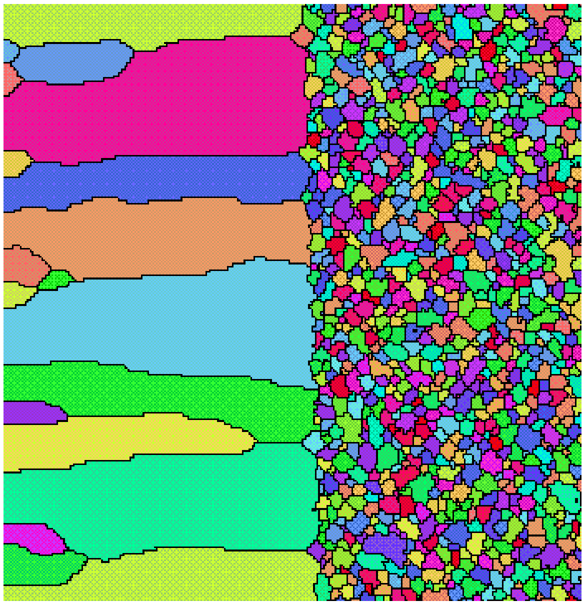
VI.I Materials Process Modeling for Microstructure Optimization

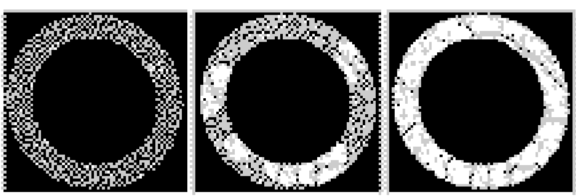
Introduction: The processing of a material can be the determining factor in it's cost and it's performance. Often a material's strength, reliability, and other properties are sensitive to details of processing. In order to reduce costs and to optimize a material's performance, materials scientists must gain a better understanding of the relationship between processing conditions and the resulting microstructure. Nearly all materials forming processes (forging, rolling, extrusion, welding, powder processing) include high-temperature excursions during which grain structure evolves, whether intentional (annealing) or inadvertent (heat affected zone in welds). Microstructural evolution can take many forms during these processes: e.g., grain growth, recrystallization, precipitation, and coarsening. These microstructural changes introduced by forming largely determine the final material properties.



Columnar grain development in zone annealing.

Calculational Notes: The calculation uses the Monte Carlo Potts model to simulate the annealing of a polycrystalline grain structure. The simulations in two dimensions involve 40,000 sites and take a day to run on a fast workstation. A prototype three-dimensional algorithm includes 64 million sites, runs on 1000 processors of ASCI-Red, and a run takes 326 seconds.

Results: The top figure shows a zone annealing simulation of a gas turbine blade alloy. The grain size in the initial, randomly oriented, microstructure is about ten microns. The figure shows the development of a creep resistant columnar grain structure, which results when the material is pulled through a highly localized hot zone (a narrow vertical region at the middle of the figure). Simulations allow determination of process parameters (pull speed, hot zone temperature) that optimize the grain aspect ratio (length and width). As another practical application, the lower figure shows the recrystallized grain structure in an incandescent lamp filament. Related simulations revealed process parameters that influence development of the creep-resistant grain structure.



Recrystallization of a tungsten lamp filament.

Significance: Simulations provide a flexible tool for probing the dependence of microstructure on a range of processing conditions. The model's reliability can be enhanced by accurate input parameters from smaller length scale models (atomic, interface, dislocation), while the model's output can be directly utilized by larger scale continuum simulations for the prediction of material performance. These microstructural evolution models will play a critical role in forging the links from materials composition to processing and from processing to performance.